Appendix D

A 1-D Diffusion Code Description

1 Requirements

The code solves the 1-D slab diffusion equation on $[0, x_0]$ with options for source or vacuum boundary conditions at either face, reflective boundary conditions at the left face, and an option for the FSDS technique with either isotropic or plane-wave boundary sources on the right face. At least 2 distinct material regions must be allowed. Cross sections and cell sizes may vary between regions, but they are constant within a region. Output must include both the scalar fluxes, and all terms appearing in the global balance expression. We assume a standard 1D grid with half-integral indexes at the cell faces and integral indices at the cell centers. All problems must be scaled so that the total source rate is unity, i.e.,

$$j_L^+ + j_R^- + \sum_{i=1}^{N} q_{d,i}\ h_i = 1.0\,, \quad p/(cm^2 - sec), \tag{1}$$

where N denotes the total number of cells, and h_i is the width of cell i.

2 First-Scattered Distributed Sources

We want to apply the FSDS approximation in our diffusion code for two types of boundary fluxes: isotropic and plane-wave.

2.1 Isotropic Case

The uncollided scalar flux for an incident isotropic boundary flux of $\frac{\phi_0}{2\pi}$ $(p/cm^2 - sec - steradian)$ at $x = x_0$ is given by

$$\phi(x) = \phi_0 E_2 \left[\sigma_t(x_0 - x)\right] , \qquad x \in [0, x_0]. \tag{2}$$

The first-scattered source for the diffusion equation is therefore

$$q_f(x) = \sigma_s \phi_0 E_2 \left[\sigma_t(x_0 - x)\right] . \tag{3}$$

In order to maintain particle conservation, it is best to define the discrete source values as follows:

$$q_i = \frac{1}{h_i} \int_{x_{i-1/2}}^{x_{i+1/2}} q(x) dx \, . \tag{4}$$

Calculating the discrete first-scattered source in accordance with Eq. (4), we get

$$q_i = \frac{1}{2} \sigma_s \phi_0 \frac{1}{h_i} \int_{x_{i-1/2}}^{x_{i+1/2}} E_2 \left[\sigma_t(x_0 - x)\right] \, dx \, . \tag{5}$$

To evaluate this integral, we note that

$$\frac{d}{dx} E_n(x) = -E_{n-1}(x) \, . \tag{6}$$

Let $\xi = \sigma_t(x_0 - x)$, then (4) can be expressed as follows:

$$\begin{aligned} q_i &= \frac{\sigma_s \phi_0}{\sigma_t h_i} \int_{\xi_{i+1/2}}^{\xi_{i-1/2}} E_2(\xi)\ d\xi\,. \\ &= \frac{\sigma_s \phi_0}{\sigma_t h_i} \Big|_{\xi_{i-1/2}}^{\xi_{i+1/2}} E_3(\xi) \\ &= \frac{\sigma_s \phi_0}{\sigma_t h_i} \left\{ E_3\left[\sigma_t(x_0 - x_{i+1/2})\right] - E_3\left[\sigma_t(x_0 - x_{i-1/2})\right] \right\}\,. \end{aligned} \tag{7}$$

2.2 Plane-Wave Case

Given a plane-wave source of $\frac{\phi_0}{2\pi}\delta(\mu+1)\quad p/(cm^2 - sec - steradian)$, the uncollided scalar flux is

$$\phi(x) = \phi_0 \exp\left[-\sigma_t(x_0 - x)\right]\,, \qquad x \in [0, x_0]\,. \tag{8}$$

The first-scattered distributed source for the diffusion equation is therefore

$$q_f(x) = \sigma_s \phi_0 \exp\left[-\sigma_t(x_0 - x)\right] \tag{9}$$

Calculating the discrete first-scattered source in accordance with Eq. (4), we get

$$\begin{aligned} q_i &= \frac{1}{h_i} \int_{x_0 - x_{i+1/2}}^{x_0 - x_{i-1/2}} \sigma_s \phi_0 \exp\left[-\sigma_t(x_0 - x)\right]\ dx \\ &= \frac{\sigma_s \phi_0}{\sigma_t h_i} \left\{ \exp\left[-\sigma_t(x_0 - x_{i+1/2})\right] - \exp\left[-\sigma_t(x_0 - x_{i-1/2})\right] \right\}\,. \end{aligned} \tag{10}$$

3 Global Particle Balance

If we integrate the diffusion equation over $[0, x_0]$, we obtain a conservation expression for the entire slab:

$$J(x_0) - J(0) + \sum_{i=1}^{N} \sigma_{a,i}\phi_i h_i = \sum_{i=1}^{N} q_i h_i \, . \tag{11}$$

The currents can be further broken down into inflows and outflows:

$$\begin{aligned} J(0) &= \left[\frac{\phi(0)}{4} + \frac{J(0)}{2}\right] - \left[\frac{\phi(0)}{4} - \frac{J(0)}{2}\right] , \\ &= j_L^+ - j_L^- , \\ &= \text{(left inflow) - left(outflow)} \, . \end{aligned} \tag{12}$$

$$\begin{aligned} J(x_0) &= \left[\frac{\phi(x_0)}{4} + \frac{J(x_0)}{2}\right] - \left[\frac{\phi(x_0)}{4} - \frac{J(x_0)}{2}\right] , \\ &= j_R^+ - j_R^- , \\ &= \text{(right outflow) - (right inflow)} \, . \end{aligned} \tag{13}$$

Putting all the expressions together, we get

$$j_R^+ + j_L^- + \sum_{i=1}^{N} \sigma_{a,i}\phi_i h_i = j_L^+ + j_R^- + \sum_{i=1}^{N} q_i h_i \, . \tag{14}$$

The left side of Eq. (14) represents sinks and the right side represents sources.

When the FSDS technique is being used, the corresponding balance expression is

$$\left(j_{U,R}^+ + j_{C,R}^+\right) + \left(j_{U,L}^- + j_{C,L}^-\right) + \sum_{i=1}^{N} \sigma_{a,i}\left(\phi_{U,i} + \phi_{C,i}\right) h_i =$$

$$\left(j_{U,L}^{+} + j_{C,L}^{+}\right) + \left(j_{U,R}^{-} + j_{C,R}^{-}\right) + \sum_{i=1}^{N} \; q_{d,i} h_i \,, \tag{15}$$

Where "U" denotes an uncollided quantity, "C" denotes a collided quantity, q_d denotes the explicit distributed source (excluding the first-scattered source), and $\phi_{C,i}$ denotes the average uncollided flux in cell i:

$$\phi_{C,i} = \frac{1}{h_i} \int_{x_{i-1/2}}^{x_{i+1/2}} \; \phi_C(x) \, dx \,. \tag{16}$$

Note that the uncollided partial currents, j_C^{+} and j_C^{-} must be exactly evaluated by angular integration of the boundary fluxes. Equations (12) and (13) apply to only the diffusion solution and not to the uncollided flux solution.